Temperature Dependence of Infinite Dilution Activity Coefficients and Henry's Law Constants of Some Polycyclic Aromatic Hydrocarbons in Water

J. Reza [C, S]
Programa de Ingeniería Molecular, Area de Investigacion en Termofisica, Instituto Mexicano del Petróleo, México D. F., Mexico

A. Trejo
Competencia de Ciencias Básicas, Instituto Mexicano del Petróleo, México D. F., Mexico

Infinite dilution activity coefficients (IDAC) and Henry's law constants (HLC) are physicochemical parameters useful to predict the distribution and fate of pollutants in the various compartments on the global environment. In addition to its significance in environmental applications, the knowledge of IDAC provides insight into the chemical and physical forces that exist between solute and solvent molecules. On the other hand, HLC are useful for designing separation and purification equipment, and to evaluate the applicability of potential regeneration and treatment methods. In this work are reported the aqueous infinite dilution activity coefficients of four polycyclic aromatic hydrocarbons (anthracene, pyrene, 9,10-dihydrophenanthrene, 9,10-dihydroanthracene), in the temperature range comprised between 278 and 323 K. The IDAC were determined from the experimental water solubility data of each polycyclic aromatic hydrocarbon, previously determined, as well as from the knowledge of their enthalpies of fusion and their heat capacities of both solid and liquid phases. The values of the IDAC obtained range from 802,000 to 24,400,000 with an average error of 9.8 per cent. These are the first reported IDAC values (as a function of temperature), for the above mentioned compounds. From the knowledge of the IDAC, and the vapor pressure of each considered polycyclic aromatic hydrocarbons (PAHs), the mole fraction-based Henry's law constants, as a function of temperature, were also calculated. These HLC were then used to derive the air-water partition coefficients (AWPC) of each studied PAH. From the dependence of AWPC with temperature, the enthalpy, entropy and Gibbs free energy related to the transference of each hydrocarbon between air and water phases were also obtained. The data presented in this work are useful to predict the environmental behavior of long-lived organic as well as to have a better understanding about the several interactions involved in the aqueous solution process of highly hydrophobic organic compounds.